



Accurate Mass: 445.170983

Percentage Composition: C 51.23%; H 5.20%; N 22.01%; O 21.55%

Physical Description: Powder; cryst. +1H₂O as hydrochloride

Solubility: Sol. H₂O

pKa Value: pK_a 1.24; pK_a 3.5; pK_a 4.8; pK_a 4.82; pK_a 10.5 (2225°, CONH₂, 22)

Hazard & Toxicity: Exp. reprod. and teratogenic effects

Fluka: 87355

Sigma: T3250

>>Derivative: 5-Formyl

>>Derivative: 5-N-Me

CAS Registry Number: 134-35-0

Extra CAS Registry Numbers(s): 26560-38-3

Biological Source: Has been used as a modulator of 5-fluorouracil toxicity in cancer patients, but effectiveness not supported by phase II clinical trials

Physical Description: Cryst. (H₂O + 2-mercaptoethanol)

Other Data: Mp >300° (as Ca salt)

References:

- May, M. *et al.*, *J.A.C.S.*, 1951, **73**, 3067-3075, (*formyl derivs*)
Kallen, R.G. *et al.*, *J. Biol. Chem.*, 1966, **24**, 5845, (*props*)
Blair, J.A. *et al.*, *Anal. Biochem.*, 1970, **34**, 376-381, (*synth, uv, pmr, N-Me*)
Ruediger, H. *et al.*, *FEBS Lett.*, 1970, **11**, 265-267, (*synth, biochem, N-Me*)
Fontecilla-Camps, J.C. *et al.*, *J.A.C.S.*, 1978, **101**, 6114, (*abs config*)
Feeney, J. *et al.*, *J.C.S. Perkin 2*, 1980, 176, (*derivs, pmr, cmr*)
Kattchee, P.A. *et al.*, *Anal. Biochem.*, 1981, **118**, 85-90, (*synth, deriv*)
Charlton, P.A. *et al.*, *J.C.S. Perkin 1*, 1985, 1349, (*synth, uv*)
Sato, J.K. *et al.*, *Anal. Biochem.*, 1986, **104**, 516, (*synth, derivs*)
Selhub, J. *et al.*, *Anal. Biochem.*, 1989, **182**, 84-93, (*anal, hplc, N-Me*)
Brunner, H. *et al.*, *Chem. Ber.*, 1992, **125**, 2085, (*synth, bibl*)
Hilhorst, E. *et al.*, *Tet. Lett.*, 1993, **34**, 4257-4260, (*biochem*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, TCR400